

Access DB#

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: 1/ Sabiha Khatun Examiner #: 74141 Date: 11/2/04
Art Unit: 1616 Phone Number: 206 222 Serial Number: 09/646327
Mail Box and Bldg Room Location: _____ Results Format Preferred (circle): PAPER DISK E-MAIL
4C7D Raw 4A45

If more than one search is submitted, please prioritize searches in order of need.

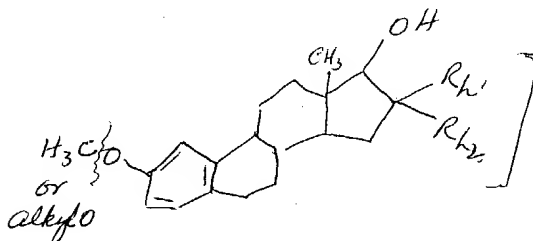
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or inquiry of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Inventors (please provide full names): Agoston et al.

Earliest Priority Filing Date: 8/18/2000.

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please Search for the Compound #
Cl 34 and its method of use



alkyl, CH_2OH ,
 $\text{CH}_2\text{N}(\text{Me})_2$.

Please see prev⁸

Thank you

See attached sheet

STAFF USE ONLY

Searcher: _____

Searcher Phone #:

Searcher Location:

Date Searched Picked Up:

Rate Completed: 11/9

Searcher Prep & Review Time: 15

Chemical Prep Time: _____

Online Page 12

Type of Search

NA Sequence (#) _____

AA Sequence (#)

Structure (//)

Bibliographic

Litigation

Fulltext

Patent Family

Other

Vendors and cost where applicable

STN 305,98

Dialog

Questel/Orbit

Dr.Link

Lexis/Nexis

Sequence Systems

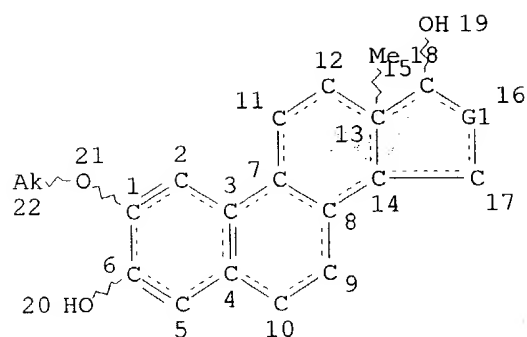
WWW/Internet

Other (specify) _____

=> d que 14

L1

STR

CH~G2
@23 24G2~C~G2
25 @26 27

Ak @28

Ak~OH
@29 30Ak~N~Ak
31 @32 33
 37
 Ak
 Ak~N~Ak
 @34 35 36

VAR G1=23/26

VAR G2=28/29/32/34

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 22

CONNECT IS E1 RC AT 28

CONNECT IS E2 RC AT 29

CONNECT IS E1 RC AT 31

CONNECT IS E1 RC AT 33

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CONNECT IS E1 RC AT 36

CONNECT IS E1 RC AT 37

DEFAULT MLEVEL IS ATOM

GGCAT IS LIN SAT AT 29

GGCAT IS LIN SAT AT 34

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

L3 15 SEA FILE=REGISTRY SSS FUL L1

L4 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d 14 ibib abs hitstr.1-5

L4 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:3558 HCAPLUS

DOCUMENT NUMBER: 140:73598

TITLE: Systems and methods for rapid evaluation and design of molecules for predicted biological activity

INVENTOR(S): Hendry, Lawrence B.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 44 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004002052	A1	20040101	US 2002-279546	20021023
PRIORITY APPLN. INFO.:			US 2001-344560P	P 20011023
			US 2001-339954P	P 20011210

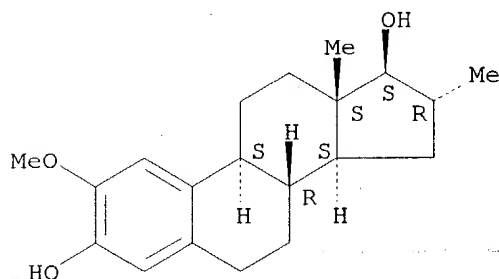
AB The computer-based systems and methods are for rapidly evaluating mols. for suspected biol. activity and relative potency, and for designing mols. for desired biol. activity. The systems and methods enable rapid screening of large mol. databases using one or more search engines designed to identify mols. predicted to possess specific biol. activities. Estradiol, 8 other estrogens and the conformation of the DNA site into which they fit were used to construct a search engine which was used to search databases containing a variety of compound structures.

IT **431901-98-3**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(as standard in construction of search engine for evaluation of substances for predicted antiangiogenic activity; systems and methods for rapid evaluation and design of mols. for predicted biol. activity)

RN 431901-98-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry:



L4 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:719252 HCAPLUS

DOCUMENT NUMBER: 139:224972

TITLE: Synthesis of 2-methoxyestradiol derivatives and uses
as antiangiogenic agents

INVENTOR(S): Lavalley, Theresa M.; Pribluda, Victor S.; Simons,
Jonathan; Mabjeesh, Nicola; Giannakakou, Paraskevi

PATENT ASSIGNEE(S): Entremed, Inc., USA

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003073985	A2	20030912	WO 2003-US5898	20030227
WO 2003073985	A3	20031231		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-361267P P 20020301

AB Comps. and methods for treating mammalian disease characterized by undesirable angiogenesis and for controlling a number of angiogenesis-related events, conditions, or substances, by administering derivs. of 2-methoxyestradiol of general formula (I) wherein the variables are defined in the specification.

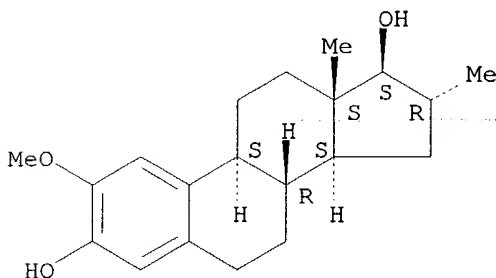
IT 431901-98-3P 431901-99-4P 431902-01-1P
 431902-02-2P 431902-03-3P 431902-04-4P
 431902-05-5P 431902-06-6P 438044-30-5P
 594873-86-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic agents)

RN 431901-98-3 HCAPLUS

CN Estradiol, 1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

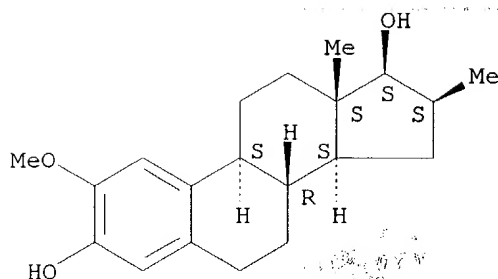
Absolute stereochemistry.



RN 431901-99-4 HCAPLUS

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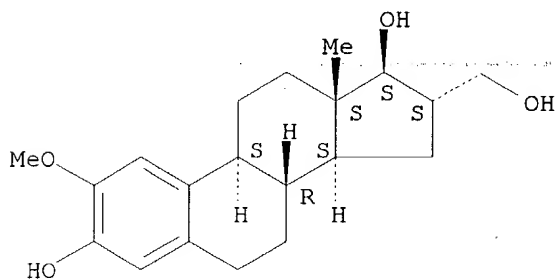
Absolute stereochemistry.



RN 431902-01-1 HCAPLUS

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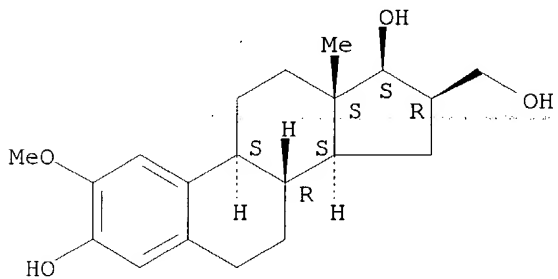
Absolute stereochemistry.



RN 431902-02-2 HCAPLUS

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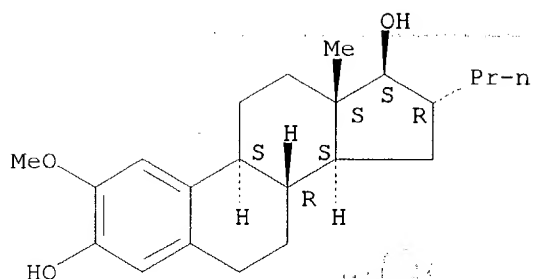
Absolute stereochemistry.



RN 431902-03-3 HCAPLUS

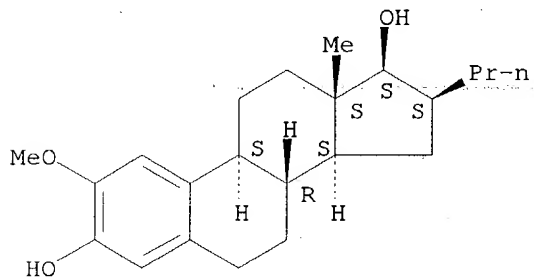
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(16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



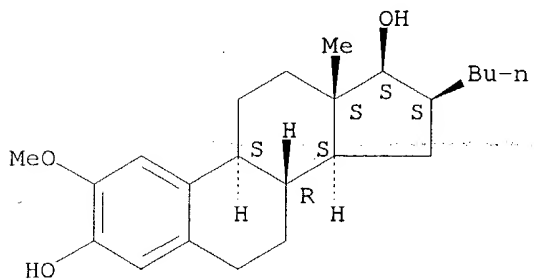
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 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



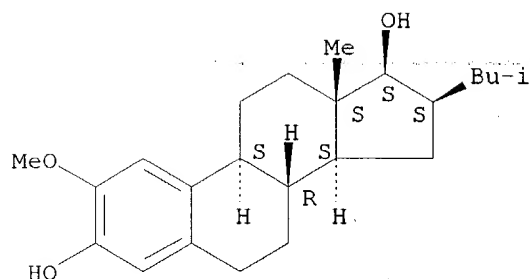
RN 431902-05-5 HCAPLUS
 CN Estradiol-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 431902-06-6 HCAPLUS
 CN Estradiol-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-(2-methylpropyl)-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

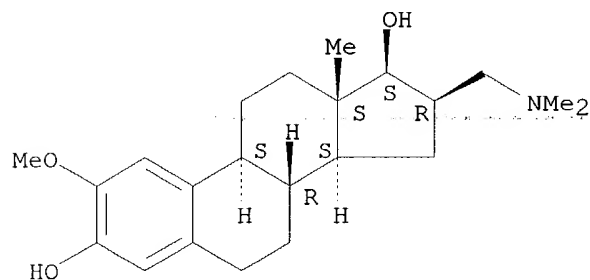
Absolute stereochemistry.



RN 438044-30-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-,
(16 β ,17 β)- (9CI) (CA INDEX NAME)

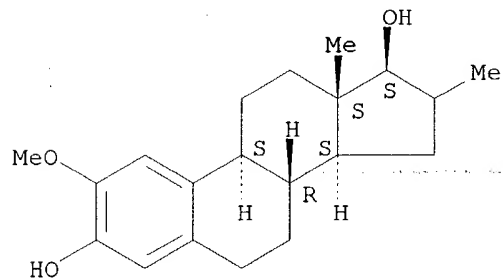
Absolute stereochemistry.



RN 594873-86-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-, (17 β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

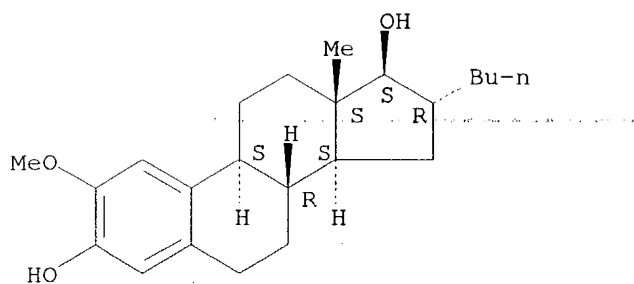
ACCESSION NUMBER: 2002:778714 HCAPLUS

DOCUMENT NUMBER: 2002:778714 137:279370

TITLE: Preparation of 2-methoxyestradiol derivatives as
antiangiogenic agents

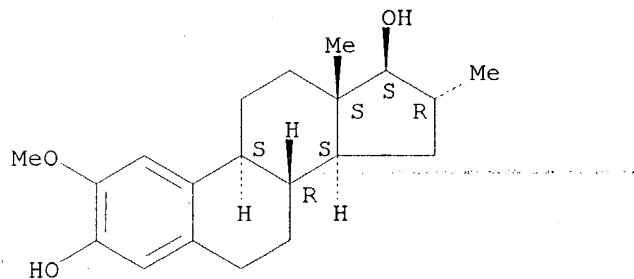
INVENTOR(S): Agoston, Gregory E.; Pribluda, Victor; Treston,
Anthony M.; Green, Shawn J.

PATENT ASSIGNEE(S): USA



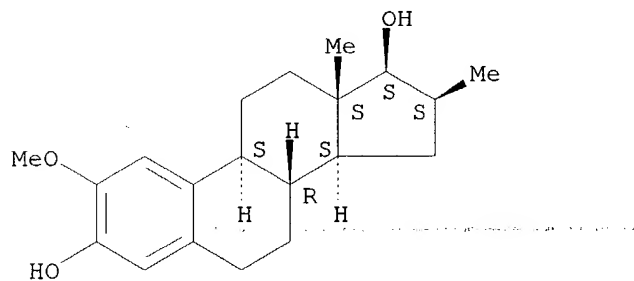
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 (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



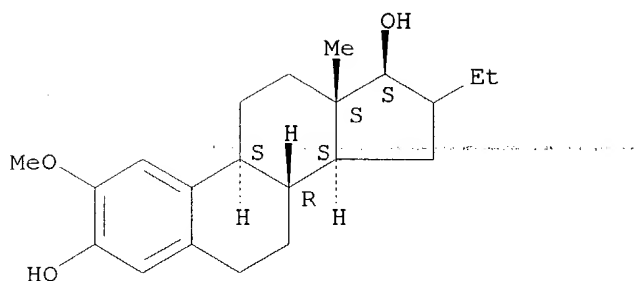
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 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



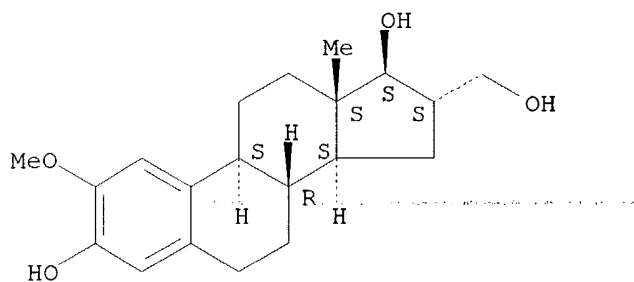
RN 431902-00-0 HCAPLUS
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 (CA INDEX NAME)

Absolute stereochemistry.



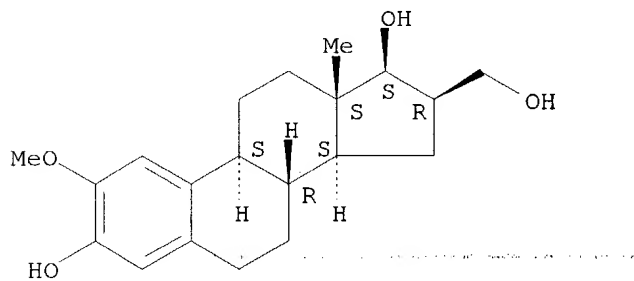
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 (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



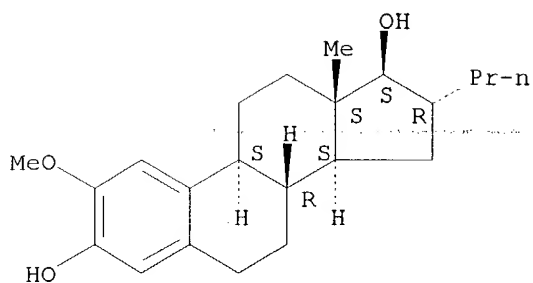
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 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



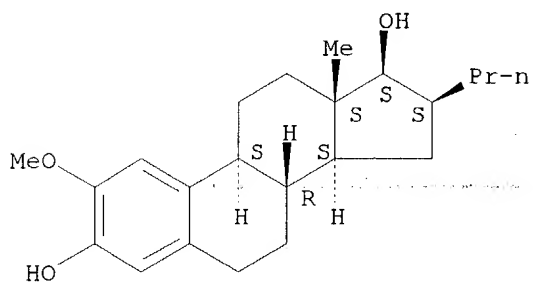
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 CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



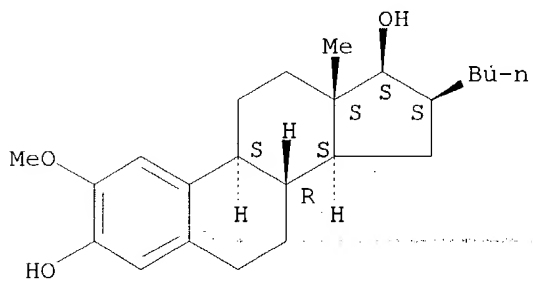
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 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



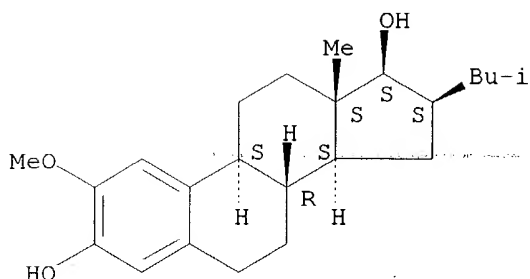
RN 431902-05-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 431902-06-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-(2-methylpropyl)-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

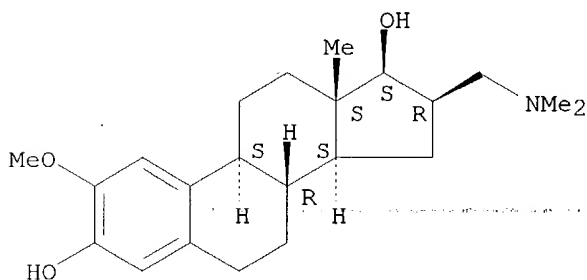
Absolute stereochemistry.



RN 438044-30-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-,
(16β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:488275 HCAPLUS

DOCUMENT NUMBER: 137:47357

TITLE: Preparation of 2-methoxyestradiol derivatives as
antiangiogenic agentsINVENTOR(S): Agoston, Gregory E.; Shah, Jamshed H.; Hunsucker,
Kimberly A.; Pribluda, Victor S.; Lavalley, Theresa
M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan,
Xiaoguo H.; Treston, Anthony M.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 37 pp., Cont.-in-part of U. S.
Ser. No. 933,894.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

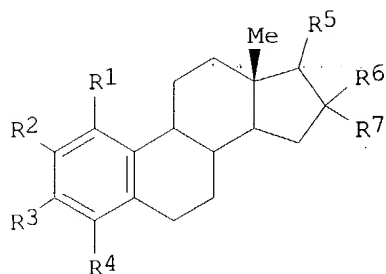
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

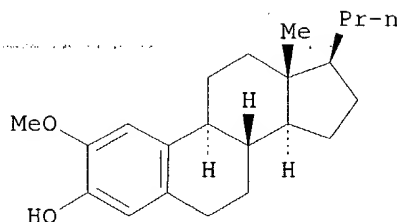
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002082433	A1	20020627	US 2001-939208	20010824
PRIORITY APPLN. INFO.:			US 2000-641327	A2 20000818
			US 2000-253385P	P 20001127
			US 2000-255302P	P 20001213
			US 2001-278250P	P 20010323
			US 2001-933894	A2 20010821

OTHER SOURCE(S):
GI

MARPAT 137:47357



I



II

AB 2-Methoxyestradiol derivs. of formula I [R1, R4 = H, halo, CN, alkyl, OH, NH2, etc.; R2 = N3, CN, OMe, alkenyl, alkynyl, alkoxy, NH2, etc.; R3 = OH, OAc; R5 = alkyl, alkenyl, (di)alkylamino, OH, alkylene, etc.; R6, R7 = H, alkyl, alkenyl, alkynyl, halo, etc.] are prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepared from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The IC50 of II against MDA-MB-231 breast tumor cells was 51.31 μ M.

IT 431901-87-0P 431901-98-3P 431901-99-4P
431902-00-0P 431902-01-1P 431902-02-2P
431902-03-3P 431902-04-4P 431902-05-5P
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438044-30-5P

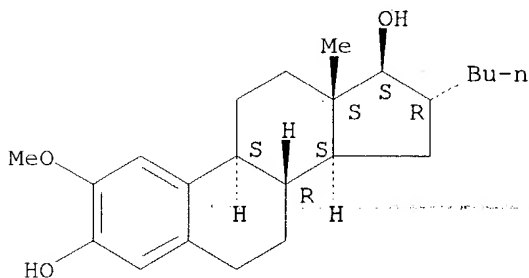
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents).

RN 431901-87-0 HCAPLUS

CN Estradiol-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

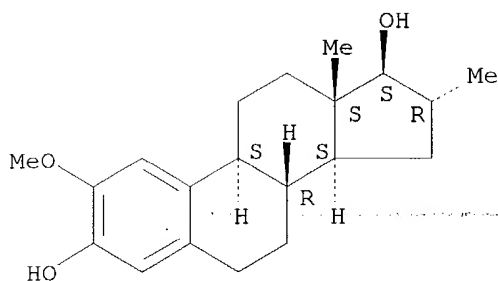
Absolute stereochemistry.



RN 431901-98-3 HCAPLUS

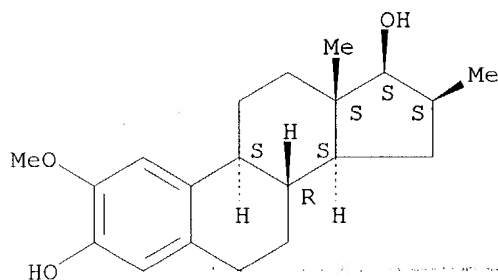
CN Estradiol-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



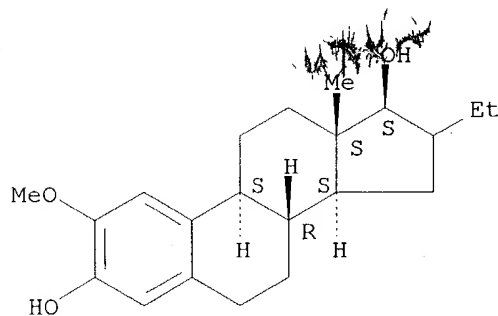
RN 431901-99-4 HCAPLUS
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 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



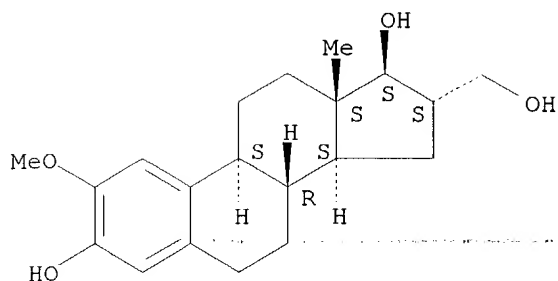
RN 431902-00-0 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-ethyl-2-methoxy-, (17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 431902-01-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

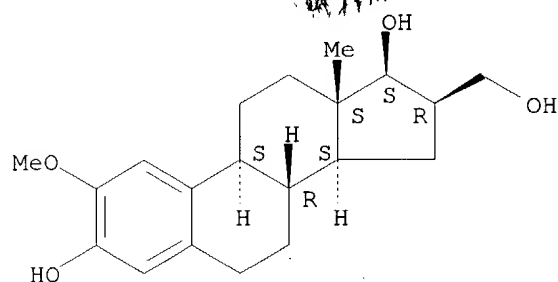
Absolute stereochemistry.



RN 431902-02-2 HCAPLUS

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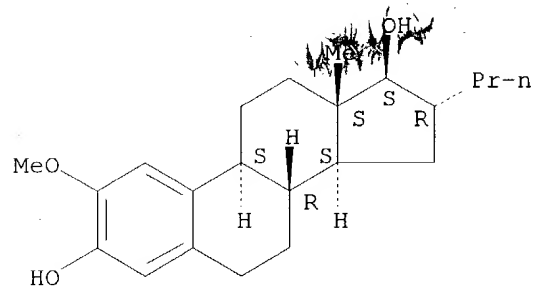
Absolute stereochemistry.



RN 431902-03-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

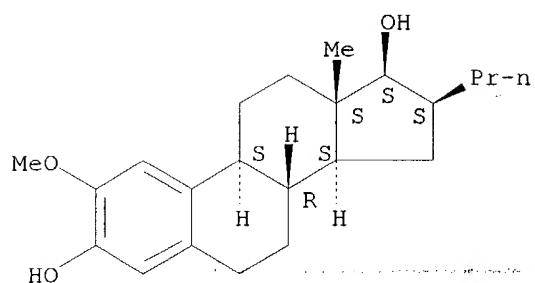
Absolute stereochemistry.



RN 431902-04-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-,
(16 β ,17 β)- (9CI) (CA INDEX NAME)

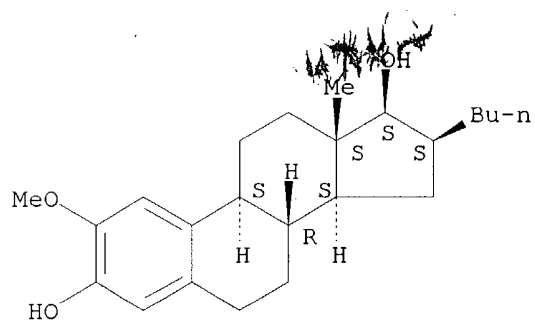
Absolute stereochemistry.



RN 431902-05-5 HCAPLUS

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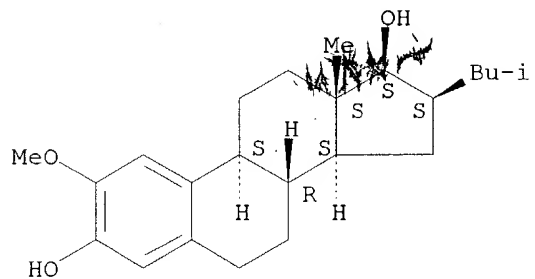
Absolute stereochemistry.



RN 431902-06-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-(2-methylpropyl)-,
(16 β ,17 β)- (9CI) (CA INDEX NAME)

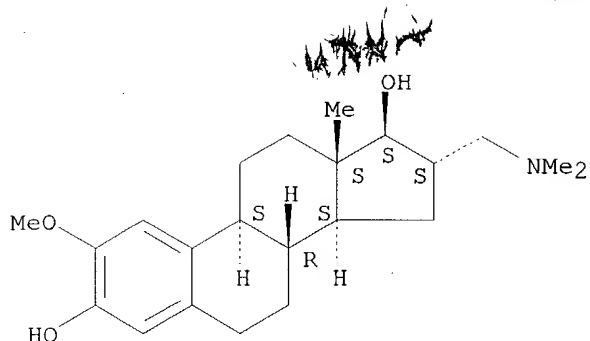
Absolute stereochemistry.



RN 431902-07-7 HCAPLUS

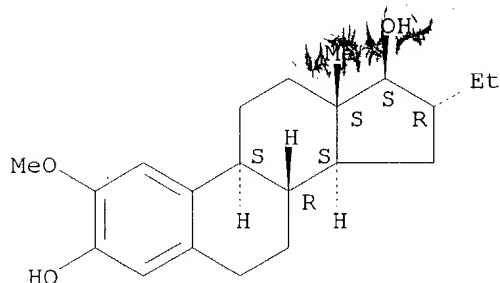
CN Estra-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



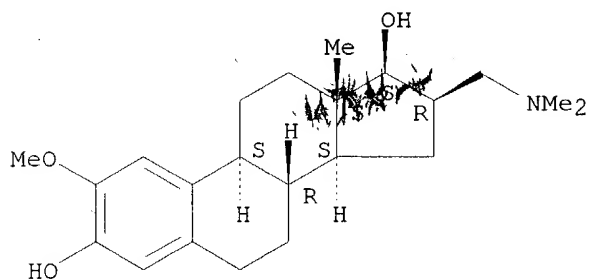
RN 431902-08-8 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-ethyl-2-methoxy-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 438044-30-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

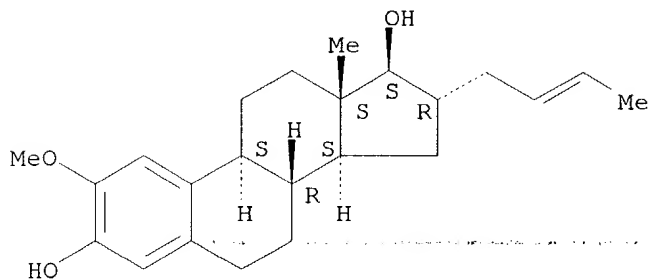
Absolute stereochemistry.



IT **438044-33-8P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)
 RN 438044-33-8 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-(2-butenyl)-2-methoxy-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



L4 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:408687 HCAPLUS

DOCUMENT NUMBER: 137:6309

TITLE: Preparation of 2-methoxyestradiol analogs as antiangiogenic agents

INVENTOR(S): Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor; Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony

PATENT ASSIGNEE(S): Entremed, Inc., USA

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

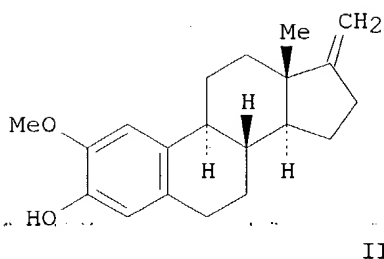
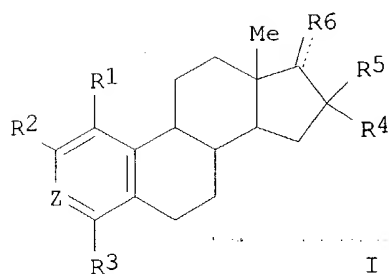
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002042319	A2	20020530	WO 2001-US26490	20010824
WO 2002042319	A3	20030313		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001088386	A5	20020603	AU 2001-88386	20010824
EP 1343803	A2	20030917	EP 2001-968112	20010824
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRIORITY APPLN. INFO.:				
			US 2000-253385P	P 20001127
			US 2000-255302P	P 20001213
			US 2001-278250P	P 20010323
			US 2001-933894	A 20010821
			WO 2001-US26490	W 20010824

OTHER SOURCE(S): MARPAT 137:6309

GI



AB 2-Methoxyestradiol analogs, such as I [R1, R3 = H, halo, CN, alkyl, OH, CH2OH, NH2, alkylamino; R2 = N3, CN, C.tplbond.CR, C=CHR, C.tplbond.CH, OR, amino; R = H, alkyl; Z = COH, COAc; dashed bond = single bond or double bond; R6 = H, OH, O, oxime, amino, alkyl, alkenyl; R4, R5 = H, alkyl, alkenyl, allyl], were prepared for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepared by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and HUVEC endothelial cells, II showed IC50 0.24±0 and 0.19±0.19 resp.

IT 431901-87-0P 431901-98-3P 431901-99-4P
 431902-00-0P 431902-01-1P 431902-02-2P
 431902-03-3P 431902-04-4P 431902-05-5P
 431902-06-6P 431902-07-7P 431902-08-8P

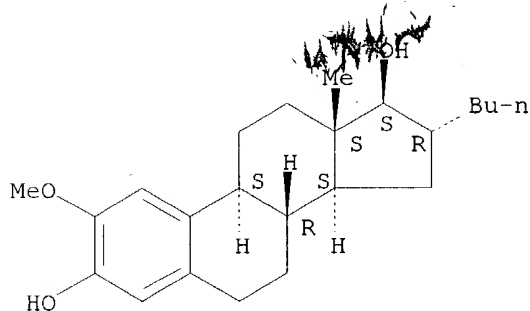
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents)

RN 431901-87-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-,
 (16α,17β)- (9CI) (CA INDEX NAME)

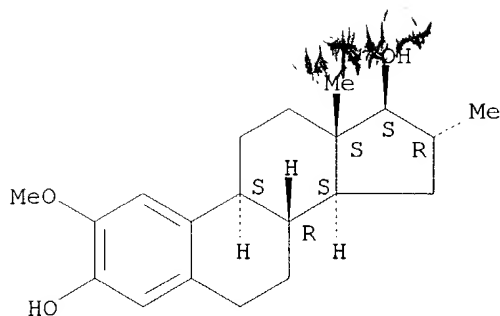
Absolute stereochemistry.



RN 431901-98-3 HCAPLUS

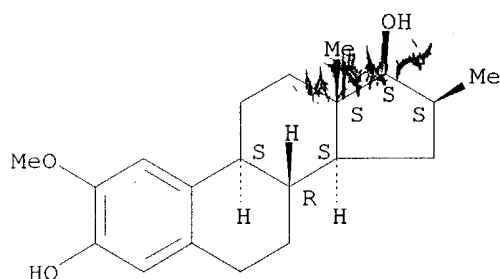
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-,
 (16α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



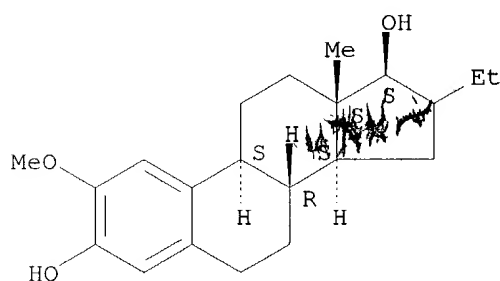
RN 431901-99-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



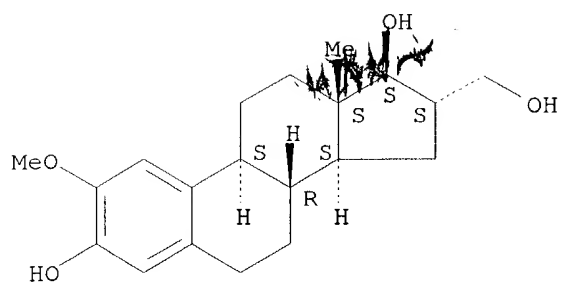
RN 431902-00-0 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-ethyl-2-methoxy-, (17 β)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 431902-01-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

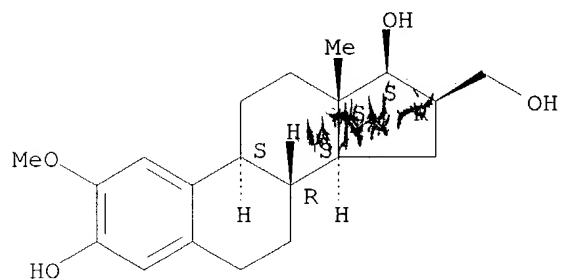
Absolute stereochemistry.



RN 431902-02-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-,
(16 β ,17 β)- (9CI) (CA INDEX NAME)

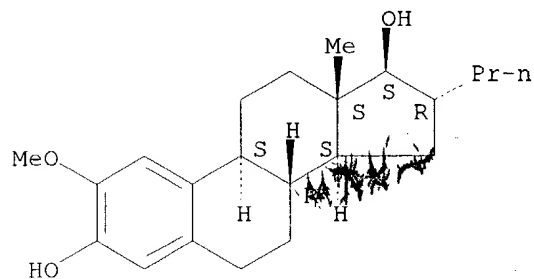
Absolute stereochemistry.



RN 431902-03-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

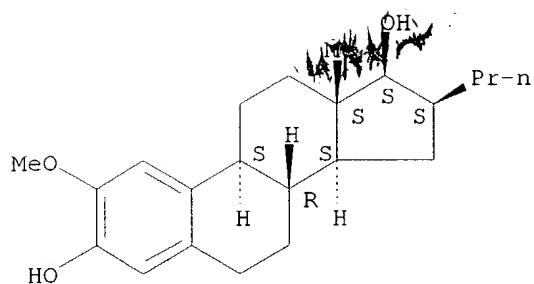
Absolute stereochemistry.



RN 431902-04-4 HCAPLUS

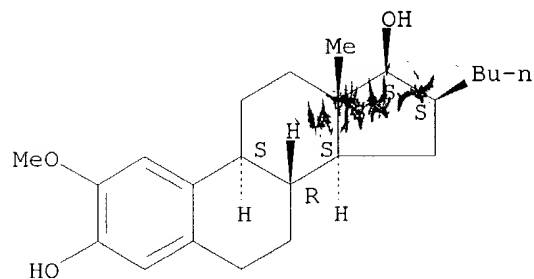
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-,
(16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



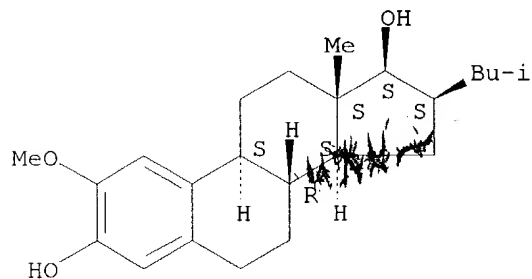
RN 431902-05-5 HCAPLUS
 CN Estradiol-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



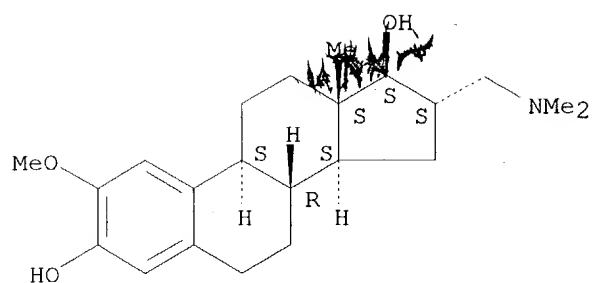
RN 431902-06-6 HCAPLUS
 CN Estradiol-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-(2-methylpropyl)-,
 (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 431902-07-7 HCAPLUS
 CN Estradiol-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-,
 (16 α ,17 β)- (9CI) (CA INDEX NAME)

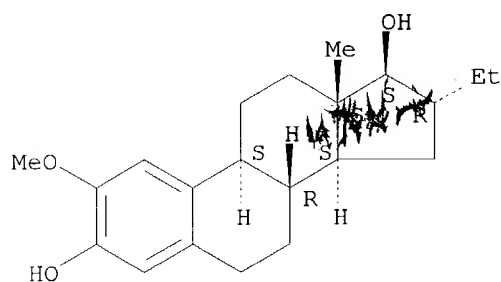
Absolute stereochemistry.



RN 431902-08-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-ethyl-2-methoxy-,
(16 α ,17 β)- (9CI) (CA INDEX NAME)

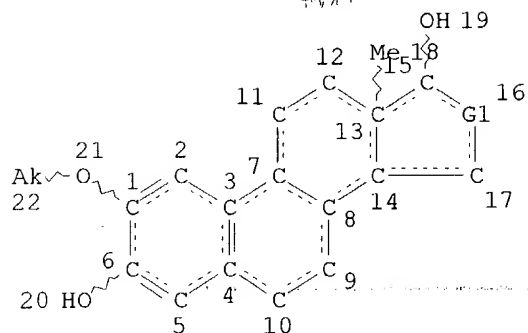
Absolute stereochemistry.



=> d que

L1

STR

CH~G2
@23 24G2~C~G2
25 @26 27

Ak @28

Ak~OH
@29 30Ak~N~Ak
31 @32 33

37
Ak
Ak~N~Ak
@34 35 36

VAR G1=23/26

VAR G2=28/29/32/34

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 22

CONNECT IS E1 RC AT 28

CONNECT IS E2 RC AT 29

CONNECT IS E1 RC AT 31

CONNECT IS E1 RC AT 33

CONNECT IS E2 RC AT 34

CONNECT IS E1 RC AT 36

CONNECT IS E1 RC AT 37

DEFAULT MLEVEL IS ATOM

GGCAT IS LIN SAT AT 29

GGCAT IS LIN SAT AT 34

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

L3 15 SEA FILE=REGISTRY SSS FUL L1

L4 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

L6 7 SEA FILE=MARPAT SSS FUL L1

L7 5 SEA FILE=MARPAT ABB=ON PLU=ON L6/COM

L8 2 SEA FILE=MARPAT ABB=ON PLU=ON L7 NOT L4

=> d l8 ibib abs qhit 1-2

L8 ANSWER 1 OF 2 MARPAT COPYRIGHT 2004 ACS on STN

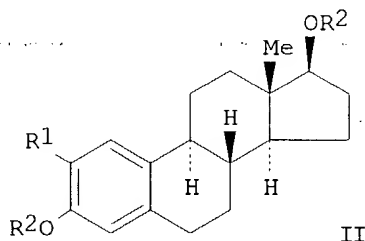
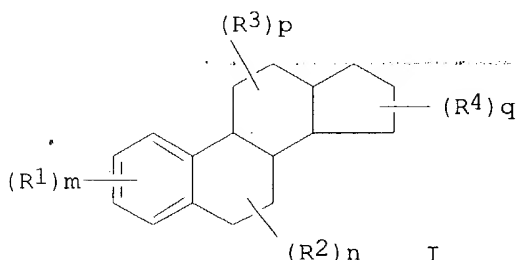
ACCESSION NUMBER: 134:295993 MARPAT

TITLE: Estradiol conjugates and their therapeutic applications

INVENTOR(S): Stewart, Alastair George; McAllister, David James;
 Collis, Maree Patricia; Robertson, Alan Duncan
 PATENT ASSIGNEE(S): University of Melbourne, Australia
 SOURCE: PCT Int. Appl., 57 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

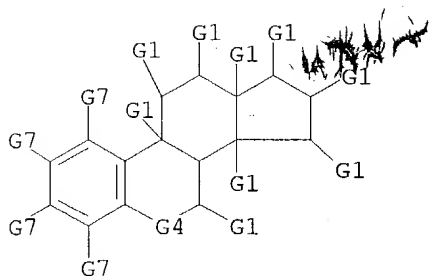
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001027132	A1	20010419	WO 2000-AU1244	20001013
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1226154	A1	20020731	EP 2000-969105	20001013
R: AT, BE, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003511461	T2	20030325	JP 2001-530350	20001013
ZA 2002002622	A	20030304	ZA 2002-2622	20020404
PRIORITY APPLN. INFO.:			AU 1999-3425	19991014
			WO 2000-AU1244	20001013

GI



AB The invention discloses the preparation of conjugated prodrug of estradiol compound I (R1-R4 = H, OH, halo, alkyl, alkenyl, alkynyl, cycloalkyl, amino, aryl, keto, hydrazono, oximino, carbohydrate, peptide, etc.; m,n,p,q = 0-3), a pharmaceutically acceptable salt or in vivo hydrolyzable ester, amide carbonate or carbamate thereof, in the treatment of conditions associated with enhanced angiogenesis or accelerated cell division, such as cancer, and inflammatory conditions such as asthma and rheumatoid arthritis and hyperproliferative skin disorders including psoriasis. Thus, II [R1 = OMe, R2 = H (III)] was prepared via multi-step reaction sequence starting from β -estradiol II (R1-R2 = H). In human airway fibroblasts thrombin-stimulated increases in cell number were reduced to $12 \pm 8\%$ of the control response by III.

MSTR 1



G1 = OH / Me
 G4 = 33

HC—G1
 33

G7 = OH / OMe
 MPL: claim 10
 NTE: or derivatives, pharmaceutically acceptable salts, or in vivo hydrolyzable esters, amides, carbonates, or carbamates
 NTE: substitution is restricted
 NTE: also incorporates claim 32, formulas IV, V, and VI

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 MARPAT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 133:150782 MARPAT

TITLE: synthesis of 16-Hydroxyestratrienes as selectively effective estrogens

INVENTOR(S): Kuenzler, Hermann; Knauth, Rudolf; Lessl, Monika; Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa; Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ,

BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2000029095 A5 20000829 AU 2000-29095 20000209
 EP 1144431 A2 20011017 EP 2000-907539 20000209
 EP 1144431 A3 20020612

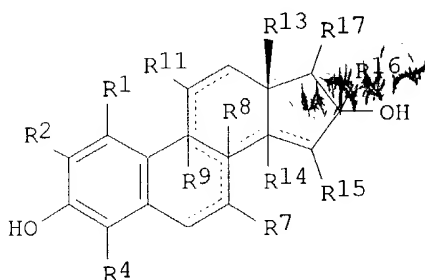
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO

BR 2000008076 A 20020205 BR 2000-8076 20000209
 JP 2002536455 T2 20021029 JP 2000-598520 20000209
 EE 200100412 A 20021216 EE 2001-412 20000209
 NZ 513409 A 20040227 NZ 2000-513409 20000209
 NO 2001003860 A 20011008 NO 2001-3860 20010808
 BG 105804 A 20020329 BG 2001-105804 20010809

PRIORITY APPLN. INFO.:

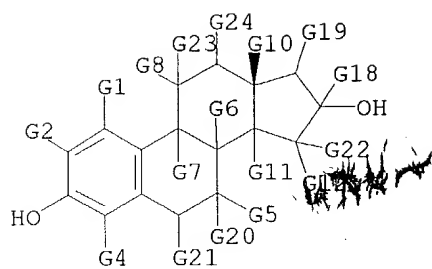
DE 1999-19906159 19990209
 WO 2000-EP1073 20000209

GI



AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2, CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16 α -estradiol shows a 50% uterine stimulation at 30 μ g in in vivo testing.

MSTR 1



G2 = 21

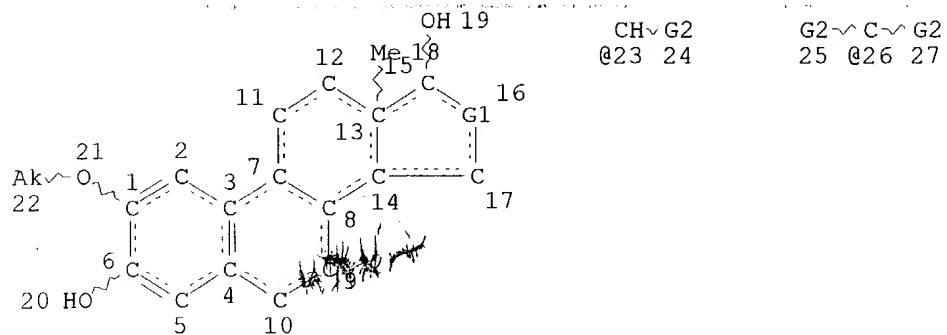
$\text{O} \text{---} \text{G3}$
21

G3 = Me
G10 = Me
G18 = Me
G19 = OH
MPL: claim 1
NTE: substitution is restricted
NTE: additional interruptions also claimed

=> d que

L1

STR



Ak @28

CH~G2
@23 24G2~C~G2
25 @26 27Ak~OH
@29 30Ak~N~Ak
31 @32 33

37
Ak
Ak~N~Ak
@34 35 36

VAR G1=23/26

VAR G2=28/29/32/34

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 22

CONNECT IS E1 RC AT 28

CONNECT IS E2 RC AT 29

CONNECT IS E1 RC AT 31

CONNECT IS E1 RC AT 33

CONNECT IS E2 RC AT 34

CONNECT IS E1 RC AT 37

DEFAULT MLEVEL IS ATOM

GGCAT IS LIN SAT AT 29

GGCAT IS LIN SAT AT 34

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE

L5 0 SEA FILE=BEILSTEIN SSS FUL L1